

Modeling work at UIUC

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Modeling efforts at the UIUC

- VFTRIM-3D modeling of solid phase lithium (with and without D-treatment), tin-lithium and tin
- VFTRIM-3D modeling of liquid phase lithium and tin-lithium
- Studies on self-sputtering of lithium as a function of angle of incidence
- Studies on temperature-dependent mechanisms on the sputtering yield of lithium
- Hydrocarbon redeposition modeling using MD code to assist erosion/redeposition studies at ANL (D. Alman)

Simulation with VFTRIM-3D for D,He and Li on solid and liquid lithium target

- Lithium in Solid Phase

50 %D, 50%Li ([H.Sugai, Vacuum, 47 6-8 \(1996\) 981](#))

$$sbe = 1.68 \text{ eV}$$

$$Be = 0.168 \text{ eV} = 10\% * SBE$$

- Lithium in Liquid Phase

In liquid state, deuterium atoms will diffuse to bulk, forming Li-D bonds in subsequent layers below

- ([R.M. Alire, J. Chem. Phys. 65, 3 \(1976\) 1134.](#))

Layer 1: 100 % Li, $sbe = 1.40 \text{ eV}$ (~10 angstroms)

Layer 2: 50%D, 50% Li with Li-Li bond energy of 1.1 eV and Li-D bond energy of 2.49 eV

Smooth surface (fractal dimension = 2.00)

Simulation with VFTRIM-3D for D,He and Li on liquid 0.8 Sn-Li target

- 0.8 Sn-Li in Liquid Phase

In liquid state, lithium atoms will segregate to the surface, with 0.8 Sn-Li in layers below.

- (R. Bastasz and W. Eckstein J. Nucl. Mater. 290-293 (2001) 19-24)

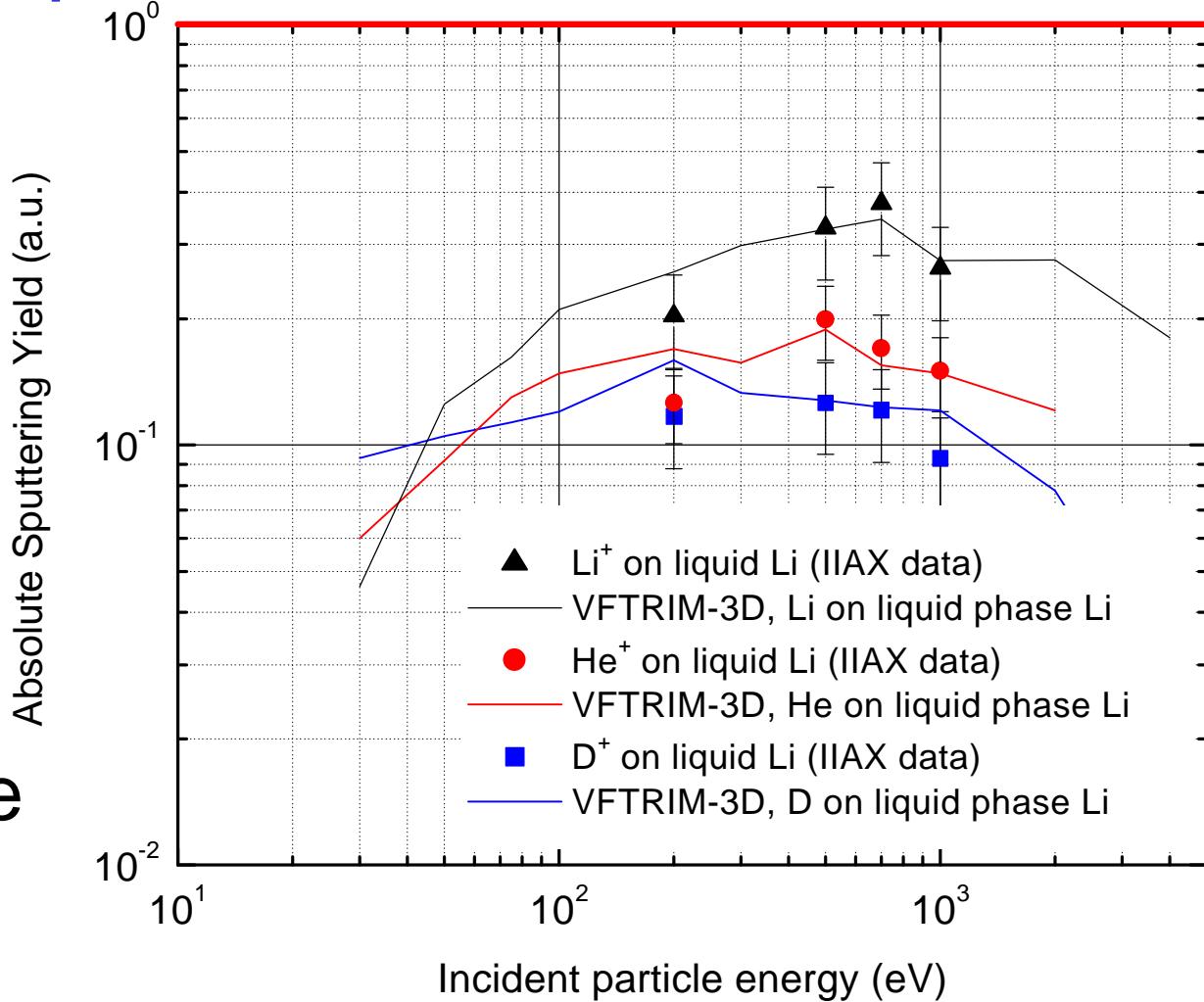
Layer 1: 100 % Li, sbe = 1.40 eV, with Li-Li bond energy of 1.1 eV

Layer 2: 20% Li, 80% Sn, sbe = 2.83, with Li-Li bond energy of 1.1 eV and Li-Sn bond energy of 0.283 eV

Smooth surface (fractal dimension = 2.00)

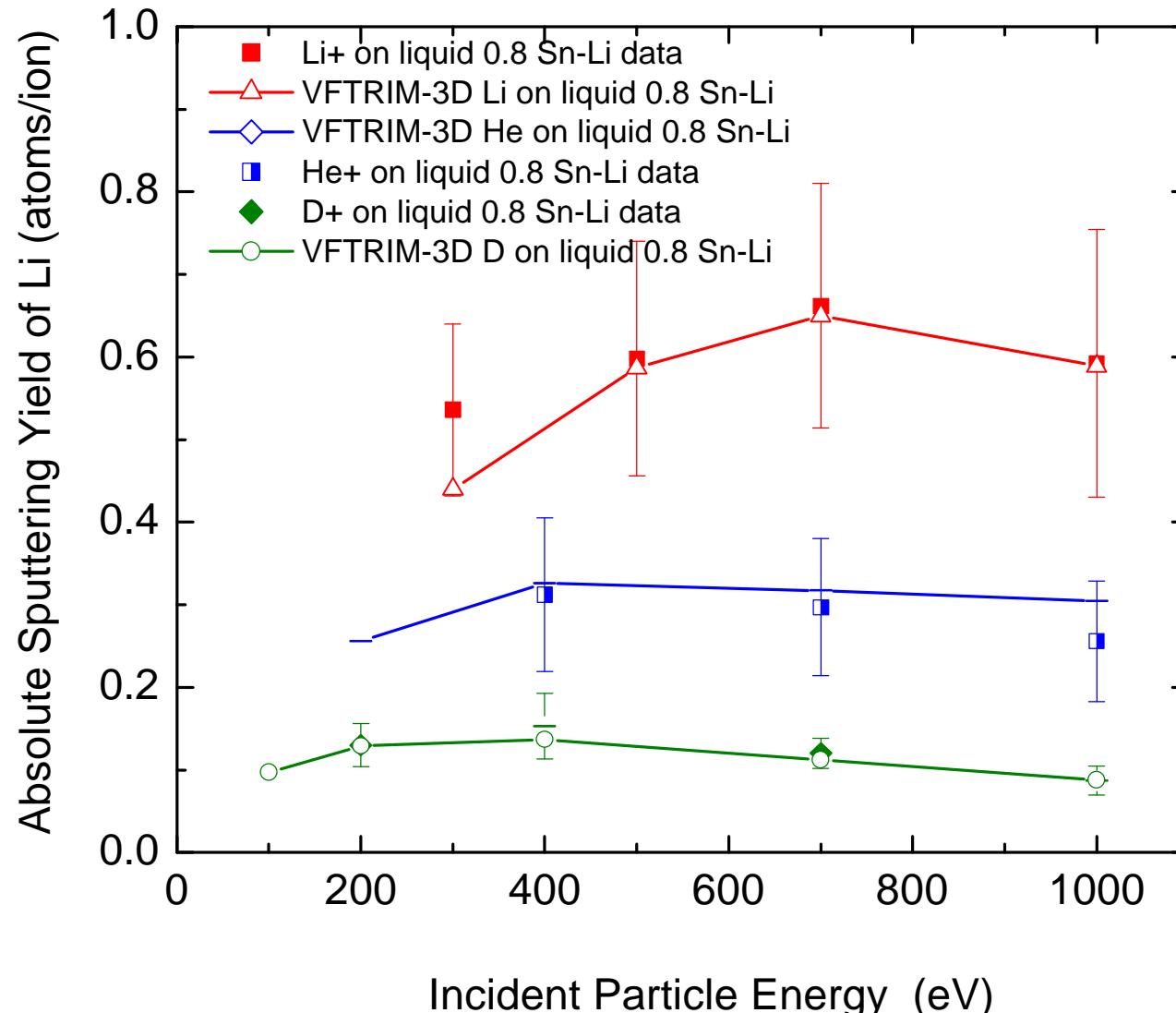
IIAX experimental and modeling data on liquid lithium erosion

- D-treated lithium yields are well below unity
- Data taken at 45 deg. Incidence and 200 °C surface temperature

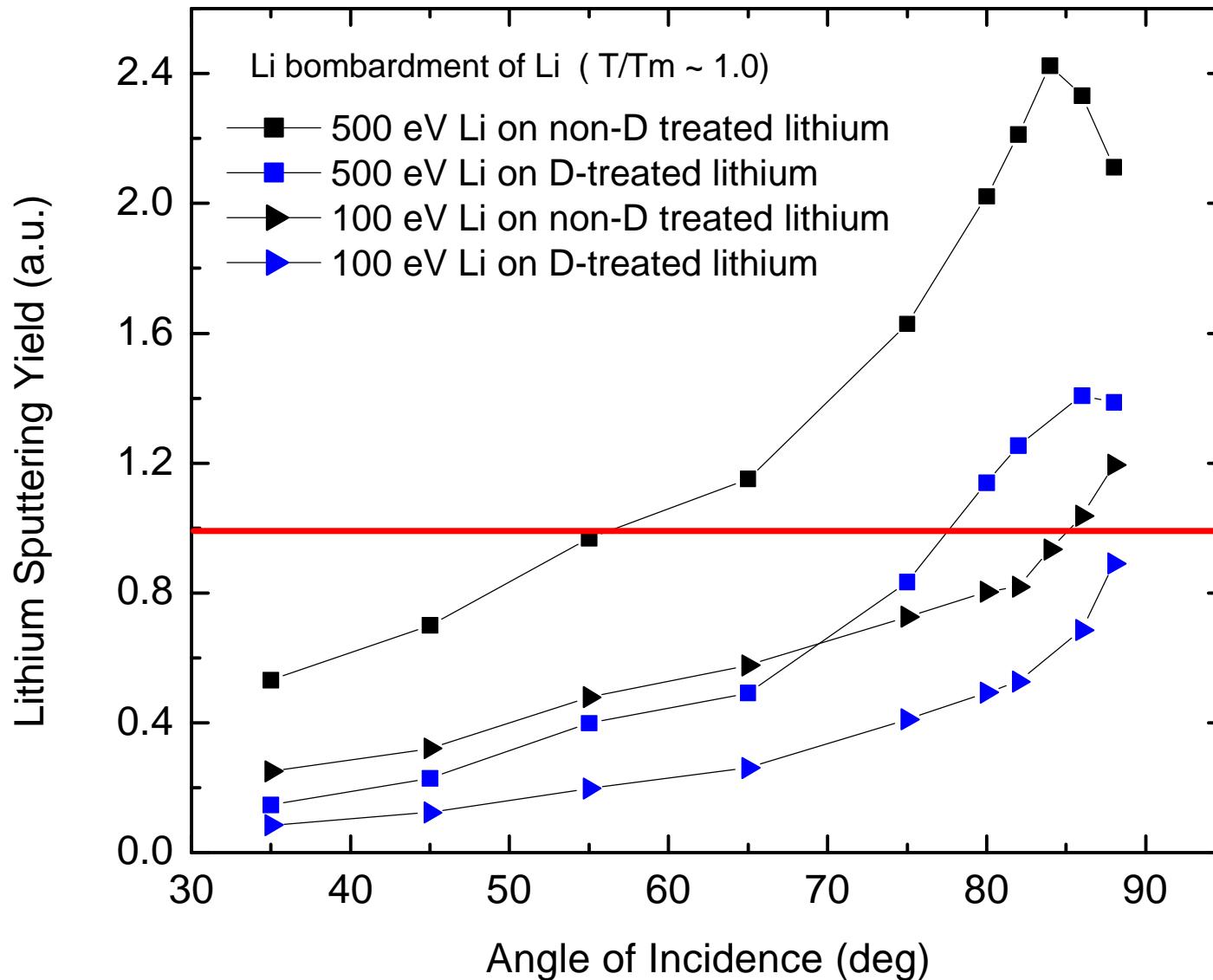


J.P. Allain, M.R. Hendricks and D.N. Ruzic, J. Nucl. Mater. 290-293 (2001) 180-184.

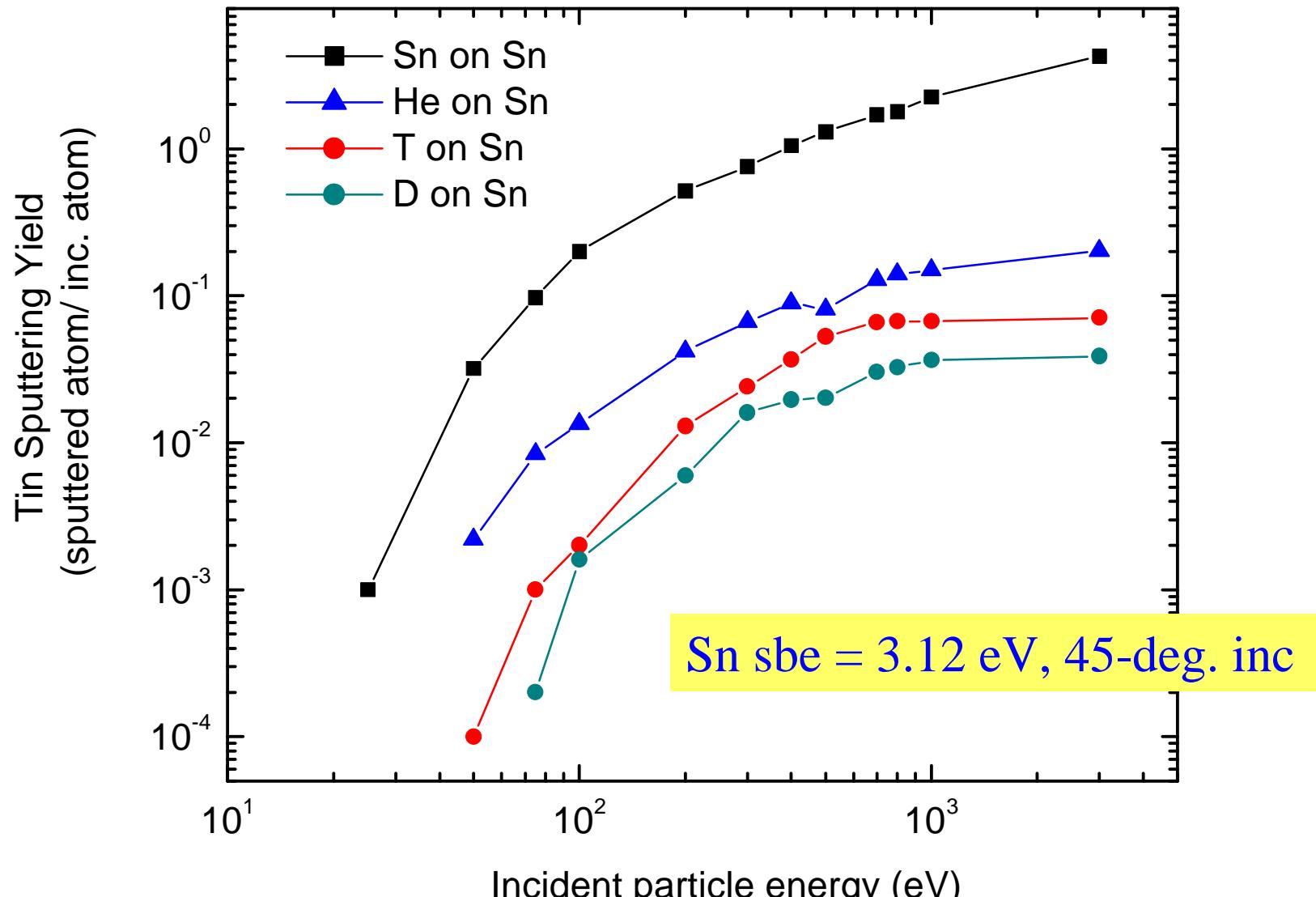
D⁺, He⁺ and Li⁺ bombardment of liquid tin-lithium data and VFTRIM-3D simulation at 45-degree incidence. (J.P. Allain, M.R. Hendricks, D.N. Ruzic, J.Nucl.Mater. 290-293 (2001) 33-37)



Total (sputtering + reflection) lithium erosion from lithium bombardment



VFTRIM-3D modeling of Sn sputtering at oblique incidence



Future Work

- Couple temperature-dependent sputtering modeling to $T/T_m > 1.0$ regime for lithium sputtering yield dependence on incident angle and incident particle energy
- Continue modeling work on Sn and calibrate to planned temperature-dependent data in IIAX
- Study angular and energy distributions of reflected and sputtered particles from hot liquid surfaces
- Continue studies on lithium segregation in liquid tin-lithium alloys